CONTENTS

Ab initio force fields of glycine dipeptide in C_5 and C_7 conformations
T.C. Cheam and S. Krimm (Ann Arbor, MI, U.S.A.) 1

IR matrix isolation studies of nucleic acid constituents: the spectrum of monomeric thymine
M.J. Nowak (Warsaw, Poland) 35

Dielectric relaxation of *N,N'*-diethylurea in non-polar media
B. Żywucki and J. Jadżyn (Poznan, Poland), M. Stockhausen and A. Steffen (Munster, F.R.G.) 51

Vibrational properties of the $YBa_2Cu_3O_{7-x}$ superconductor. Part I. Infrared and Raman scattering spectra: librational mechanism of superconductivity
J. Hanuza, J. Klamut, R. Horyń and B. Jeżowska-Trzebiatowska (Wroclaw, Poland) 57

The torsional motion and thermodynamic properties of biphenyl
Z. Bereszynski and L. Sobczyk (Wroclaw, Poland) and M. Pawlikowski (Kraków, Poland) .. 73

Crystallographic studies and physicochemical properties of π-electron systems. Part XVIII. Crystal and molecular structure of *N*-n-propyl-quinoxalinium 7,7',8,8'-tetracyano-*p*-quinodimethanide: estimation of charge at TCNQ by the HOSE model
K. Woźniak and T.M. Krygowski (Warsaw, Poland) 81

FTIR spectra of adsorbed n-butylamine
G. Ramis and G. Busca (Genova, Italy) 93

Water in krypton matrices
A. Engdahl and B. Nelander (Lund, Sweden) 101

Synthesis and crystal structure of a 1:1:1 adduct of *N,N'*-di(*m*-tolyl)piperazine *N,N'*-dioxide, acetic acid and water
C.-K. Kwok and T.C.W. Mak (Hong Kong) 111

The effects of phenyl substituents on the geometry and charge density of vinylacetylene
R. Destro, F. Merati and E. Ortoleva (Milan, Italy) 121

A dipole moment study of hindered benzophenones
H. Lumbroso and Ch. Liégeois (Paris, France), G. Goethals and R. Uzan (Amiens, France) .. 133

Structural studies of di-Schiff bases with a middle flexible group, relationship between the structure and liquid crystal properties
P. Cerrada, M. Marcos and J.L. Serrano (Zaragoza, Spain) and C. Jaime (Barcelona, Spain) 147

Conformational study of N-substituted 9-azabicyclo[3.3.1]nonan-3-ones
M.S. Arias, I. Iriepa, E. Galvez and A. Lorente (Madrid, Spain) 161

Fluorimetric and theoretical study of the rotamerism of *trans*-styrylanthracenes
G. Bartocci, F. Masetti and U. Mazzucato (Perugia, Italy), I. Baraldi (Modena, Italy) and E. Fischer (Rehovot, Israel) 173

^{1}H NMR spectra of the all-*trans*, 7-*cis*, 9-*cis*, 13-*cis* and 15-*cis* isomers of β-carotene: elongation of the double bond and shortening of the single bond toward the center of the conjugated chain as revealed by vicinal coupling constants
Y. Koyama, M. Hosomi and H. Hashimoto (Nishinomiya, Japan) and T. Shimamura (Ibaraki, Japan) 185

Model calculations for mixed alkali metal halide microclusters
F. Ramondo, L. Bencivenni and V. Rossi (Rome, Italy) 203

Infrared gas phase band contour separations: theoretical verification of empirical relations and deduction of new separation relations
B.J. van der Veken and P. Coppens (Antwerp, Belgium) 211

Infrared and ultraviolet investigation of the conformation and proton acceptor ability of 2,2'-pyridil
P. Migchels, G. Maes and Th. Zeegers-Huyskens (Heverlee, Belgium) and M. Rospenk (Wroclaw, Poland) 223

The geometric structures of the disulphur difluoride isomers: an experimental and ab initio study
C.J. Marsden (Parkville, Victoria, Australia), H. Oberhammer (Tübingen, F.R.G.), O. Lösking and H. Willner (Hannover, F.R.G.) 233
Hydrogen bonding. Part 27. Amine/hydrogen fluoride molecular complexes
R.R. Lovelace and K.M. Harmon (Rochester, MI, U.S.A.) 247
Conformational analysis of polyfunctional amino compounds by molecular mechanics. Part II. 1,2-Ethanediamine, 1,3-propanediamine and 1,4-diazacyclohexanes
L. Carballeira, R.A. Mosquera, M.A. Rios and C.A. Tovar (Galicia, Spain) 263
The molecular structure of silyl cyanide, determined in the gas phase by electron diffraction, microwave spectroscopy and high resolution infra-red spectroscopy, in solution in a nematic phase by NMR spectroscopy, and in the crystalline phase at 100 K by X-ray crystallography
P.D. Blair, A.J. Blake, R.W. Cockman, S. Cradock, E.A.V. Ebsworth and D.W.H. Rankin (Edinburgh, Gt. Britain) 279

Short communications
On the determination of uranium–oxygen bond lengths in dioxouranium(VI) compounds by Raman spectroscopy
J.R. Bartlett (Menai, N.S.W., Australia) and R.P. Cooney (Auckland, New Zealand) 295
Microwave spectrum and r_s coordinates of fluorobenzene-2d
M. Onda, K. Suga and I. Yamaguchi (Tokyo, Japan) 301
A simple electrostatic model for predicting the HF bond lengthening on formation of B···HF
A.C. Legon (Exeter, Gt. Britain) and D.J. Millen (London, Gt. Britain) 303
Conformational analysis of 4-methyl-1-pentyne
G.A. Crowder (Canyon, TX, U.S.A.) 307

Book Reviews 313
Announcement 319
Author Index 321
Subject Index 323